1. A method for evaluating the ability of a compound to associate with a molecule or molecular complex comprising a non-ligand binding site of an integrin βA domain, the method comprising:

(a) employing computational means to perform a fitting operation between the compound and β tail domain (βTD) contact region on the strand-F/α7 loop of an unliganded integrin (e.g., αVβ3); and

(b) analyzing the results of the fitting operation to quantify said association potential.

2. The method of claim 1 wherein the compound mimics the interaction of a peptide, comprising the amino acid sequence $C^{663}VVRFQYYE^{671}D^{672}S^{673}S^{674}G^{675}KSILYVVEEPEC^{687}$ or a fragment thereof, or $K^{618}KFDREPYMTENTCNR^{633}YCRD$ or a fragment thereof, with the strand-F/α7 loop of a βA domain of the integrin.

3. A method for identifying a candidate selective modulator of the activity of an integrin, the method comprising:

(a) modeling test compounds that fit spatially and preferentially into a βA domain non-ligand binding site of an integrin of interest using an atomic structural model of the integrin βA domain, wherein the atomic structural model is generated using amino acid sequence comprising $C^{663}VVRFQYYE^{671}D^{672}S^{673}S^{674}G^{675}KSILYVVEEPEC^{687}$ or a fragment thereof, or $K^{618}KFDREPYMTENTCNR^{633}YCRD$ or fragment thereof;

(b) screening test compounds in a biological assay for integrin activation characterized by binding of a test compound to the βA domain non-ligand binding site of the integrin; and

(c) identifying a test compound that selectively modulates the activity of the integrin, and optionally,

(d) screening an identified test compound in a biological assay for its ability to prevent interaction of the βA domain and the βTD domain by binding of the identified test compound to the βA domain non-ligand binding site of the integrin, and

(e) identifying the screened test compound as a compound capable of selectively modulating the activity of an integrin from the pool of test compounds. In various embodiments: the modulating comprises inhibiting the integrin activation and the modulating comprises inhibiting ligand binding to the integrin.

4. A method of identifying a candidate inhibitor of the activity of an integrin, the method comprising:

(a) introducing into a suitable computer program information defining a non-ligand binding site of an integrin βA domain, the information comprising a conformation defined by the coordinate atoms as in Table 1 or Table 2 or both as defined in Figures 9 and 10, wherein the program displays the three-dimensional structure thereof;

(b) creating a three dimensional structure of a test compound in the computer program;

(c) superimposing the model of the test compound on the model of the non-ligand binding site of the integrin βA domain; and

(d) assessing whether the test compound model fits spatially into the non-ligand binding site.

5. The method of claim 4 wherein the atoms are selected from those in Table 1 and Table 2.

6. A method for identifying a candidate integrin modulating compound, the method comprising:

(a) generating a three-dimensional structure of the βTD contact region of strand-F/α7 loop of an βA domain of a non-ligand bound integrin;

(b) employing the three dimensional structure to design or select the candidate integrin modulating compound, and

(c) identifying said candidate integrin modulating compound by the data obtained by steps (a) and (b).

7. The method of claim 6 further comprising (d) providing the integrin modulating compound; and (e) determining the ability of the integrin inhibitor to bind to the integrin by contacting the modulating compound with the integrin.

8. A method for identifying a candidate integrin modulating compound, the method comprising:

(a) expressing recombinant integrin fragments containing βA domain and βTD domains; and

(b) employing the protein-protein interaction of these two domains to in screening assays to identify modulators of the βA domain and βTD domain interaction.

9. The method of claim 8 further comprising: (c) providing the integrin modulating compound; and

(d) determining the ability of the integrin modulator to bind to the integrin by measuring the interaction of the modulating compound with the integrin; and (e) using the modulating compound as a basis for drug design.

10. A method of inhibiting activation of an integrin the method comprising contacting a compound with an integrin thereby locking the βA domain structure of the integrin into a non-activatable form.

11. The method of claim 10 wherein the compound mimics an intrachain ligand in its interaction with the integrin.

12. The method of claim 10 wherein the intrachain ligand comprises the sequence of SEQ ID No:1, or a fragment thereof, or SEQ ID No. 2, or a fragment thereof.

13. The method of claim 10 wherein the intrachain ligand is a member of the statin family.

14. A method of identifying an integrin modulator comprising:

(a) selecting a potential inhibitor by performing rational drug design with the three-dimensional structural coordinates of Table 1 or Table 2 or both as define in Figures 9 and 10, wherein selecting is performed in conjunction with computer modeling;

(b) contacting the potential inhibitor with an integrin domain; and

(c) detecting the ability of the potential inhibitor for inhibiting the integrin.

15. The method of claim 14 wherein step (c) is performed using a ligand binding assay.

16. The method of claim 14 wherein step (c) is performed using a cellular-based assay.

17. The method of claim 16 further comprising:

(d) growing a supplemental crystal comprising a complex formed between the integrin domain and a first potential inhibitor from step (a), the supplemental crystal effectively diffracts X-rays for the atomic coordinates of the complex a resolution of greater than 4.0 Å;

(e) determining the three-dimensional structure of the supplemental crystal;

(f) selecting a second potential inhibitor by performing rational drug design with the three-dimensional structure determined for the supplemental crystal, wherein selecting is performed in conjunction with computer modeling;

(g) contacting the second potential inhibitor with the integrin domain; and

(h) detecting the ability of the second potential inhibitor for inhibiting the integrin.

18. A compound identified by the method of claim 3 with the proviso that the compound is not lovastatin.

19. A pharmaceutical compositions comprising such compounds and a pharmaceutically acceptable carrier.

20. A method for modulating, inhibiting or stimulating binding of ligands or associated proteins to integrins by modifying the interaction of integrin beta-A domain (βA) with the beta-tail domain (βTD).

21. The method of claim 20 wherein the integrin is selected from the group consisting of: αVβ1, αVβ3, αVβ5, αVβ6, αVβ8, α3β1, α4β1, α5β1, α6β1, α6β4, α7β1, α9β1, α4β7, gp3b3a, α1β1, α2β1, α10β1, α11β1, LFA-1, MAC-1, and α150β95.

22. The method of claim 20 wherein the interaction of βA with βTD is investigated using either computational or biochemical or biophysical techniques.

23. The method of claim 20 wherein either βA, βTD or both serve as structures on which the computational or biochemical or biophysical techniques are based.

24. A method for evaluating the ability of a compound to associate with a molecule or molecular complex comprising a non-ligand binding site of an integrin βA domain, the method comprising:

(a) constructing a computer model of the binding site defined by structure coordinates wherein the root mean square deviation between the structure coordinates and the structure coordinates of the amino acids of Table 1 or Table 2 according to FIGs. 9 and 10 is not more than about 4.0 Å;

(b) selecting a compound to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into the compound, (ii) selecting a compound from a small molecule database, (iii) de novo ligand design of the compound, and (iv) modifying a known inhibitor, or a portion thereof, of a protein kinase;

(c) employing computational means to perform a fitting program operation between computer models of the compound to be evaluated and the binding site in order to provide an energy-minimized configuration of the compound in the binding site; and

(d) evaluating the results of the fitting operation to quantify the association between the said compound and the binding site, whereby evaluating the ability of the compound to associate with the binding site.

25. The method according to claim 24, wherein the binding site is further defined by the structure coordinates of one or more of SEQ ID NO:1-4 amino acids according to FIGS. 9 and 10.

26. The method according to claim 24 wherein said molecule or molecular complex is defined by the set of structure coordinates for SEQ ID NO:1-4 amino acids according to FIGS. 9 and 10.

27. The method of claim 24 wherein the root mean square deviation is not more than 3 Å.

28. The method of claim 24 wherein the root mean square deviation is not more than 2.5 Å.

29. The method of claim 24 wherein the root mean square deviation is not more than 2 Å.

30. The method of claim 24 wherein the root mean square deviation is not more than 1.5 Å.

31. A method for identifying an activator or inhibitor of an integrin a non-ligand binding site of an integrin βA domain, the method comprising:

(a) constructing a computer model of the binding site defined by structure coordinates wherein the root mean square deviation between the structure coordinates and the structure coordinates of the amino acids of Table 1 or Table 2 according to FIGs. 9 and 10 is not more than about 4.0 Å;

(b) selecting a compound to be evaluated as a potential activator or inhibitor by a method selected from the group consisting of (i) assembling molecular fragments into the compound, (ii) selecting the compound from a small molecule database, (iii) de novo ligand design of the compound, and (iv) modifying a known inhibitor, or a portion thereof, of an integrin;

(c) employing computational means to perform a fitting program operation between computer models of the compound to be evaluated and the binding site in order to provide an energy-minimized configuration of the compound in the binding site;

(d) evaluating the results of the fitting operation to quantity the association between the compound and the binding site model, whereby evaluating the ability of the the compound to associate with the said binding pocket;

(e) providing the compound; and

(f) contacting the compound with the molecule to determine the ability of the compound to activate or inhibit the molecule.

32. The method according to claim 31, wherein the binding site is further defined by the structure coordinates of one or more of SEQ ID NO:1-4 amino acids according to FIGS. 9 and 10.

33. The method according to claim 31 wherein said molecule or molecular complex is defined by the set of structure coordinates for SEQ ID NO:1-4 amino acids according to FIGS. 9 and 10.

34. The method of claim 31 wherein the root mean square deviation is not more than 3 Å.

35. The method of claim 31 wherein the root mean square deviation is not more than 2.5 Å.

36. The method of claim 31 wherein the root mean square deviation is not more than 2 Å.

37. The method of claim 31 wherein the root mean square deviation is not more than 1.5 Å.